

Urea, 1-(p-fluorophenyl)-
659-30-3 | DTXSID20216106

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.84	0.55	0.85	0.53	0.83	0.64

Model Results

Predicted value: 3.78

Global applicability domain: Inside

Local applicability domain index: 5.08e-01

Confidence level: 8.37e-01

Nearest Neighbors from the Training Set

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2,2-Dimethylpropane-1,3-diol

Measured: 4.68

Predicted: 4.44

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1,1'-Oxybis-2-propanol

Measured: 4.57

Predicted: 3.83

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Sulfolane

Measured: 7.08

Predicted: 6.91

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Paraldehyde

Measured: 3.02

Predicted: 2.77

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Trimethyl phosphate

Measured: 1.41

Predicted: 1.50